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II—Two-Step Method

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Solution of Elliptic Partial Differential Equations by Fast Poisson Solvers Using a Local Relaxation Factor

II—Two-Step Method

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Summary

A two-step semidirect procedure is developed to accelerate the one-step procedure described in NASA TP-2529. For a set of constant coefficient model problems, the acceleration factor increases from 1 to 2 as the one-step procedure convergence rate decreases from $+\infty$ to 0. It is also shown numerically that the two-step procedure can substantially accelerate the convergence of the numerical solution of many partial differential equations (PDE's) with variable coefficients.

Introduction

The iterative procedure developed in reference 1 requires only a single application of a fast direct solver (FDS) in advancing u^n to u^{n+1}. In the present report the following two-step iterative procedure is investigated:

$$Pw^n = -\tau(Qu^n - h) \qquad (\tau \neq 0) \tag{1}$$

and

$$P(u^{n+1} - u^n) = Rw^n \tag{2}$$

With the understanding that the notations defined in reference 1 are used in the present report, the only parameters in equations (1) and (2) yet to be defined are w^n, the intermediate iterative variable, and R, an elliptic linear operator whose exact form will be chosen to accelerate the convergence. With the assumptions that (1) $u^n \to u$ and $w^n \to w$ as $n \to +\infty$, and (2) the inverse of R exists, it may be concluded that $w = 0$ and u is a solution of equation (I-1). (Here, as in the following, the equation number (I-1), for example, refers to eq. (1) of ref. 1.)

If one assumes that the computational effort required to advance u^n *to* u^{n+1} with the two-step procedure is twice that required with the one-step procedure, the former has no merit unless it can achieve a convergence rate at least twice that of the latter. Fortunately, for a large class of the operator Q an operator R can be found such that the two-step method convergence rate is 2 to 4 times that of the one-step method convergence rate. Moreover, as will be shown, the higher acceleration factor is realized whenever the one-step method convergence rate is lower.

In the section Analysis the convergence of the two-step procedure is investigated in a fashion similar to that presented in the section Analysis of reference 1. In the section Local Relaxation the results obtained in the section Analysis are extended to solve partial differential equations (PDE's) with variable coefficients. Finally, in the section Numerical Evaluation the two-step method is numerically compared with the one-step method by using two-dimensional (2-D) and three-dimensional (3-D) test problems.

Analysis

In this section the two-step procedure defined in equations (1) and (2) is studied by assuming that τ is a constant and

$$R \overset{\text{def.}}{=} a'\frac{\partial^2}{\partial x^2} + 2b'\frac{\partial^2}{\partial x \partial y} + c'\frac{\partial^2}{\partial y^2} \tag{3}$$

where a', b', and c' are constant coefficients to be determined later. Furthermore it is assumed that the operators Q and P are those defined in equations (I-3) to (I-5). The central difference forms of equations (1) and (2) can be expressed as

$$\tilde{P}\left(w_{i,j}^n\right) = -\tau\left[\tilde{Q}\left(u_{i,j}^n\right) - h_{i,j}\right] \tag{4}$$

and

$$\tilde{P}\left(u_{i,j}^{n+1} - u_{i,j}^n\right) = \tilde{R}\left(w_{i,j}^n\right) \tag{5}$$

respectively. Here $\tilde{Q}$ and $\tilde{P}$, respectively, are defined in equations (I-8) and (I-9), and

$$\begin{aligned}\tilde{R}(v_{i,j}) \overset{\text{def.}}{=} {} & a'(\Delta x)^{-2}(v_{i+1,j} + v_{i-1,j} - 2v_{i,j}) \\ & + c'(\Delta y)^{-2}(v_{i,j+1} + v_{i,j-1} - 2v_{i,j}) \\ & + b'(2\Delta x \Delta y)^{-1}(v_{i+1,j+1} + v_{i-1,j-1} \\ & - v_{i+1,j-1} - v_{i-1,j+1})\end{aligned} \tag{6}$$

for any $v_{i,j}$.

This report has been reprinted so that the graphs of figures 1, 2, 4, and 5 are in the correct locations.

To study the convergence rate of the iterative procedure defined by equations (4) and (5), one notes that equations (4), (5), and (I-6) imply that

$$\widetilde{P}\left(w_{i,j}^{n}\right) = -\tau\widetilde{Q}\left(e_{i,j}^{n}\right) \tag{7}$$

and

$$\widetilde{P}\left(e_{i,j}^{n+1} - e_{i,j}^{n}\right) = \widetilde{R}\left(w_{i,j}^{n}\right) \tag{8}$$

where $e_{i,j}^{n}$ is defined in equation (I-11). With the assumption that both $w_{i,j}^{n}$'s and $e_{i,j}^{n}$'s satisfy the periodic and uniqueness conditions as given in equations (I-12) to (I-14), a line of arguments similar to that presented in appendix A of reference 1 can be used to show that the unique solution $e_{i,j}^{n}$ to equations (7) and (8) is

$$e_{i,j}^{n} = \sum_{(k,\ell)\in\Psi} \left[\underline{\underline{G}}^{(k,\ell)}(\tau)\right]^{n} \bullet E^{0,(k,\ell)} \bullet \varphi_{i,j}^{(k,\ell)}$$

$$(n = 1,2,3,\ldots;\ i,j = 0,\ \pm 1,\ \pm 2,\ldots) \tag{9}$$

where

$$\underline{\underline{G}}^{(k,\ell)}(\tau) \overset{\text{def.}}{=} 1 - \tau\left(\gamma^{(k,\ell)} \bullet \gamma'^{(k,\ell)}\right) \qquad (k,\ell) \in \Psi \tag{10}$$

The only parameter in equations (9) and (10) yet to be defined is

$$\gamma'^{(k,\ell)} \overset{\text{def.}}{=} \left(\frac{\sigma_r^{(k,\ell)}}{\sigma_p^{(k,\ell)}}\right) \qquad (k,\ell) \in \Psi \tag{11}$$

where

$$\sigma_r^{(k,\ell)} \overset{\text{def.}}{=} -4\left\{a'\left[\frac{1}{\Delta x}\sin\left(\frac{\pi k}{K}\right)\right]^2 + c'\left[\frac{1}{\Delta y}\sin\left(\frac{\pi\ell}{L}\right)\right]^2 + 2b'\left[\frac{1}{\Delta x}\sin\left(\frac{\pi k}{K}\right)\right] \bullet \left[\frac{1}{\Delta y}\sin\left(\frac{\pi\ell}{L}\right)\right]\cos\left(\frac{\pi k}{K}\right)\cos\left(\frac{\pi\ell}{L}\right)\right\}$$

$$(k=0,1,2,\ldots,(K-1);\ \ell=0,1,2,\ldots,(L-1)) \tag{12}$$

Note that here, as in the following, the symbol = is used to designate a parameter for the two-step procedure in case this parameter is different from its counterpart in the one-step procedure.

At this juncture note that equation (9) is identical to equation (I-21) except that $G^{(k,\ell)}(\tau)$ in equation (I-21) is replaced by $\underline{\underline{G}}^{(k,\ell)}(\tau)$ in equation (9). Thus for the two-step procedure the counterpart of equation (I-26) is

$$M^{\infty} = \underline{\underline{G}}(\tau) \tag{13}$$

where

$$\underline{\underline{G}}(\tau) \overset{\text{def.}}{=} \underset{(k,\ell)\in\Psi}{\mathrm{Max}}\left\{\left|\underline{\underline{G}}^{(k,\ell)}(\tau)\right|\right\} \tag{14}$$

Furthermore the only difference between $G^{(k,\ell)}(\tau)$ and $\underline{\underline{G}}^{(k,\ell)}(\tau)$ is that the parameter

$$\gamma^{(k,\ell)} \overset{\text{def.}}{=} \left(\frac{\sigma_q^{(k,\ell)}}{\sigma_p^{(k,\ell)}}\right)$$

in $G^{(k,\ell)}(\tau)$ is replaced by the parameter

$$\underline{\underline{\gamma}}^{(k,\ell)} \overset{\text{def.}}{=} \gamma^{(k,\ell)} \bullet \gamma'^{(k,\ell)} \qquad (k,\ell) \in \Psi \tag{15}$$

in $\underline{\underline{G}}^{(k,\ell)}(\tau)$.

Let

$$\left.\begin{array}{l} a' > 0 \\ c' > 0 \\ a'c' - (b')^2 > 0 \end{array}\right\} \tag{16}$$

and

$$\left.\begin{aligned}\hat{a}' &\overset{\text{def.}}{=} \frac{a'}{a_o}\\ \hat{c}' &\overset{\text{def.}}{=} \frac{c'}{c_o}\\ \hat{b}' &\overset{\text{def.}}{=} \frac{b'}{\sqrt{a_o c_o}}\end{aligned}\right\} \tag{17}$$

A line of arguments which leads to equation (I-B18) can be used to show that

$$\lambda'_{max} \geq \gamma'^{(k,\ell)} \geq \lambda'_{min} > 0 \qquad (k,\ell) \in \Psi \tag{18}$$

where

$$\lambda'_{max} \overset{\text{def.}}{=} \frac{1}{2}\left[\hat{a}' + \hat{c}' + \sqrt{(\hat{a}' - \hat{c}')^2 + 4(\hat{b}')^2}\right] \tag{19}$$

and

$$\lambda'_{min} \overset{\text{def.}}{=} \frac{1}{2}\left[\hat{a}' + \hat{c}' - \sqrt{(\hat{a}' - \hat{c}')^2 + 4(\hat{b}')^2}\right] \tag{20}$$

Let

$$\left.\begin{aligned}\underline{\underline{\gamma}}_{max} &\overset{\text{def.}}{=} \operatorname*{Max}_{(k,\ell)\in\Psi}\left\{\underline{\underline{\gamma}}^{(k,\ell)}\right\}\\ &\text{and}\\ \underline{\underline{\gamma}}_{min} &\overset{\text{def.}}{=} \operatorname*{Min}_{(k,\ell)\in\Psi}\left\{\underline{\underline{\gamma}}^{(k,\ell)}\right\}\end{aligned}\right\} \tag{21}$$

then equations (18) and (I-B18) imply that $\underline{\underline{\gamma}}_{max} \geq \underline{\underline{\gamma}}_{min} > 0$. As a result one may conclude that (see equations (I-27) to (I-29)) $\underline{\underline{G}}(\tau)$ reaches its minimum

$$\underline{\underline{G}}^o \overset{\text{def.}}{=} \underline{\underline{G}}(\underline{\underline{\tau}}^o) = \frac{\underline{\underline{\Sigma}} - 1}{\underline{\underline{\Sigma}} + 1} < 1 \tag{22}$$

when

$$\tau = \underline{\underline{\tau}}^o \overset{\text{def.}}{=} \frac{2}{\underline{\underline{\gamma}}_{max} + \underline{\underline{\gamma}}_{min}} \tag{23}$$

Here $\underline{\underline{\tau}}^o$ is the optimal relaxation factor for the two-step method, and

$$\underline{\underline{\Sigma}} \overset{\text{def.}}{=} \frac{\underline{\underline{\gamma}}_{max}}{\underline{\underline{\gamma}}_{min}} \geq 1 \tag{24}$$

With the assumption $\tau = \underline{\underline{\tau}}^o$, it can be concluded from equations (13) and (22) that (1) $M^\infty < 1$ and (2) M^∞ increases with an increase of $\underline{\underline{\Sigma}}$.

If the coefficients a, b, c, a_o, and c_o; the aspect ratio $(\Delta y/\Delta x)$; and the integers K and L are known, the parameter $\underline{\underline{\Sigma}}$ is a function of the coefficients a', b', and c'. Since the convergence rate increases with a decrease of $\underline{\underline{\Sigma}}$, ideally the coefficients a', b', and c' should be chosen such that $\underline{\underline{\Sigma}}$ is at its minimum. Unfortunately this optimization problem is too complicated to be solved by a simple analytical technique; thus, a simplified version of this optimization problem is solved.

To proceed, one notes that $\underline{\underline{\Sigma}}$ can be considered as a function of K and L if the parameters a, b, c, a', b', c', a_o, c_o, and $(\Delta y/\Delta x)$ are known. In the appendix the existence of

$$\underline{\underline{\Sigma}}^{\infty} \overset{\text{def.}}{=} \operatorname*{Sup}_{K\geq 2, L\geq 2}\left\{\underline{\underline{\Sigma}}\right\} \tag{25}$$

is established for any given set of a, b, c, a', b', c', a_o, c_o, and $(\Delta y/\Delta x)$. Note that in this report and reference 1 supremum and infimum of a finite set are denoted by Max and Min, respectively. On the other hand, supremum and infimum of an *infinite* set are denoted by Sup and Inf, respectively. Let

$$\underline{\underline{\Sigma}}^{*} \overset{\text{def.}}{=} \frac{(\lambda_{max} + \lambda_{min})^2}{4\,\lambda_{max}\lambda_{min}} = \frac{(\hat{a} + \hat{c})^2}{4(\hat{a}\hat{c} - \hat{b}^2)} \tag{26}$$

where λ_{max}, λ_{min}, $\hat{a}$, $\hat{b}$, and $\hat{c}$ are defined in equations (I-30) to (I-32). It is shown in the appendix that (1) $\underline{\underline{\Sigma}}^\infty \geq \underline{\underline{\Sigma}}^*$ and (2) $\underline{\underline{\Sigma}}^\infty = \underline{\underline{\Sigma}}^*$ if and only if

$$\hat{D}\hat{D}' = \Lambda I \qquad (\Lambda > 0) \tag{27}$$

where I is the 2×2 identity matrix,

$$\left.\begin{aligned}\hat{D} &\overset{\text{def.}}{=} \begin{pmatrix}\hat{a} & \hat{b}\\ \hat{b} & \hat{c}\end{pmatrix}\\ \hat{D}' &\overset{\text{def.}}{=} \begin{pmatrix}\hat{a}' & \hat{b}'\\ \hat{b}' & \hat{c}'\end{pmatrix}\end{aligned}\right\} \tag{28}$$

and Λ an arbitrary positive scalar. In this report the values of a', b', and c' are determined by using equation (27) with the assumption $\Lambda = 1$. Thus,

$$\left.\begin{aligned} a' &= \frac{a_o \hat{c}}{\hat{a}\hat{c} - \hat{b}^2} \\ c' &= \frac{c_o \hat{a}}{\hat{a}\hat{c} - \hat{b}^2} \\ b' &= \frac{-\sqrt{a_o c_o}\,\hat{b}}{\hat{a}\hat{c} - \hat{b}^2} \end{aligned}\right\} \tag{29}$$

Equation (29) obviously is consistent with equations (I-4) and (16).

With the coefficients a', b', and c' specified according to equation (29) it is shown in the appendix that

$$\underline{\underline{\Sigma}}^* \geq \underline{\underline{\gamma}}_{max} \geq \underline{\underline{\gamma}}_{min} \geq 1 \tag{30}$$

and

$$\left.\begin{aligned} \lim_{K,L \to +\infty} \underline{\underline{\gamma}}_{max} &= \underline{\underline{\Sigma}}^* \\ \lim_{K,L \to +\infty} \underline{\underline{\gamma}}_{min} &= 1 \end{aligned}\right\} \tag{31}$$

Thus, in the limit of K and $L \to +\infty$ the parameters $\underline{\underline{\tau}}^o$ and $\underline{\underline{G}}^o$, respectively, approach

$$\underline{\underline{\tau}}^* \overset{\text{def.}}{=} \frac{2}{\underline{\underline{\Sigma}}^* + 1} \tag{32}$$

and

$$\underline{\underline{G}}^* \overset{\text{def.}}{=} \frac{\underline{\underline{\Sigma}}^* - 1}{\underline{\underline{\Sigma}}^* + 1} < 1 \tag{33}$$

If equations (33), (26), (I-36), and (I-37) are used, it can be shown that

$$\underline{\underline{G}}^* = \rho(G^*) \overset{\text{def.}}{=} \frac{(G^*)^2}{2 - (G^*)^2} \tag{34}$$

Since

$$\frac{d\rho}{dG^*} = \frac{4G^*}{[2 - (G^*)^2]^2} > 0 \tag{35}$$

for $1 > G^* > 0$, one concludes that ρ is a simple monotonically increasing function of G^*. Thus, the same value of c_o/a_o which optimizes G^* (see equations (I-39) and (I-40)) will also optimize $\underline{\underline{G}}^*$. In other words the value of $\underline{\underline{G}}^*$ reaches its minimum

$$\underline{\underline{G}}^*_{min} \overset{\text{def.}}{=} \frac{(G^*_{min})^2}{2 - (G^*_{min})^2} = \frac{b^2}{2ac - b^2} \tag{36}$$

when $c_o/a_o = c/a$.

In the limit of K and $L \to +\infty$ the parameters G^* and $\underline{\underline{G}}^*$ are the asymptotic error multiplication factors for the one- and two-step methods, respectively. Assuming that the execution of one iteration in the two-step procedure requires twice as much computational time as that in the one-step procedure, one may conclude that asymptotically the two-step method is faster than the one-step method by a factor of ξ if

$$\underline{\underline{G}}^* = (G^*)^{2\xi} \qquad (1 > G^* > 0)$$

With the aid of equation (34) one obtains

$$\xi = \xi(G^*) \overset{\text{def.}}{=} 1 - \frac{\ln[2 - (G^*)^2]}{\ln[(G^*)^2]} \qquad (1 > G^* > 0) \tag{37}$$

Since

$$\frac{d\xi(x)}{dx} > 0 \qquad (1 > x > 0) \tag{38}$$

and

$$\left.\begin{aligned} \lim_{x \to 0^+} \xi(x) &= 1 \\ \lim_{x \to 1^-} \xi(x) &= 2 \end{aligned}\right\} \tag{39}$$

the acceleration factor ξ increases from 1 to 2 monotonically as the value of G^* increases from 0 to 1; that is, the higher value of ξ is realized whenever the need to accelerate the one-step method is greater. (See also fig. 1.)

In a fashion similar to that described in the section Analysis of reference 1, the two-step procedure described in this section can be generalized for a space of higher dimension. However, it should be noted that in an N-dimensional space ($N > 2$) the generalized version of equation (27) represents only a subset of the general solution to the condition $\underline{\underline{\Sigma}}^* = \underline{\underline{\Sigma}}^\infty$ (ref. 2).

Local Relaxation

With the technique of local relaxation developed in the section Local Relaxation of reference 1, the two-step procedure described in the section Analysis can be extended to solve

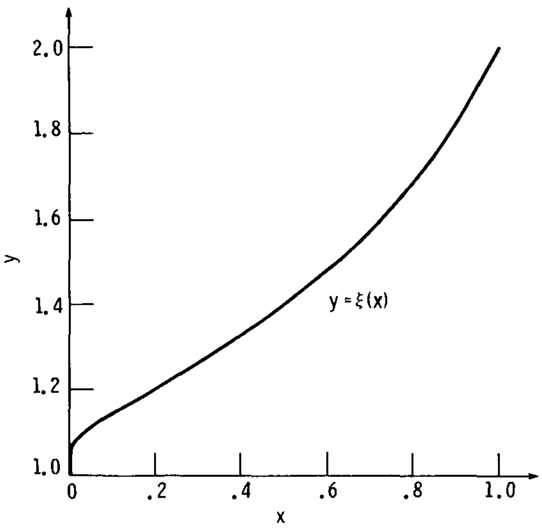

Figure 1.—Function $\xi(x) = 1 - [\ln(2 - x^2)]/(\ln x^2)$.

PDE's with variable coefficients (VC's). Thus, with the aid of equations (26) and (32) one concludes that equations (I-47) and (I-58) are replaced by

$$\underline{\underline{\tau}}_{ij} = 2 \bullet \left\{ 1 + \frac{(\hat{a}_{ij} + \hat{c}_{ij})^2}{4\left[\hat{a}_{ij}\hat{c}_{ij} - (\hat{b}_{ij})^2\right]} \right\}^{-1} \tag{40}$$

and

$$\underline{\underline{\tau}}_{ij} = 2 \bullet \left[1 + \frac{(\hat{p}_{ij} + \hat{q}_{ij})^2}{4\hat{p}_{ij}\hat{q}_{ij}} \right]^{-1} \tag{41}$$

in the two-step procedure.

Moreover, the VC versions of equations (6) and (29) are obtained by substituting the coefficients a', b', c', $\hat{a}'$, $\hat{b}'$, and $\hat{c}'$, with a'_{ij}, b'_{ij}, c'_{ij}, $\hat{a}_{ij}$, $\hat{b}_{ij}$, and $\hat{c}_{ij}$. For the case when the operator Q is a self-adjoint operator defined in equation (I-56), these VC versions are modified by replacing $\hat{a}_{ij}$, $\hat{c}_{ij}$, and $\hat{b}_{ij}$ with $\hat{p}_{ij}$, $\hat{q}_{ij}$, and 0. It should be cautioned that for the special case where $\hat{p}_{ij} = \hat{q}_{ij}$

$$\tilde{R}\left(w^n_{i,j}\right) = \frac{\tilde{P}\left(w^n_{i,j}\right)}{\hat{p}_{ij}}$$

$$\underline{\underline{\tau}}_{ij} = 1$$

$$\tau_{ij} = \frac{1}{\hat{p}_{ij}}$$

Thus, the VC versions of equations (4) and (5) imply that

$$\tilde{P}\left(u^{n+1}_{i,j} - u^n_{i,j}\right) = -\tau_{ij}\left[\tilde{Q}\left(u^n_{i,j}\right) - h_{ij}\right]$$

In other words the extra computational effort required for the two-step method is completely wasted, since the convergence achieved in one iteration is identical for both the one- and two-step methods. Note that a similar situation also arises in the solution of the PDE's with constant coefficients. Let $\hat{a} = \hat{c}$ and $\hat{b} = 0$. Then $G^* = \underline{\underline{G}}^* = 0$. In other words the machine accuracy solution is obtained in one iteration for both the one- and two-step methods. Since the parameter ξ is ill defined at $G^* = 0$ (eq. (37)), the assertion made in the section Analysis concerning the advantage of using the two-step method apparently is not valid for the special case in which $\hat{a} = \hat{c}$ and $\hat{b} = 0$.

Finally, it is noted that equations (34), (35), and (I-52) to (I-55) can be used to show that

$$(1)\ M^\infty \approx \underline{\underline{G}}^\infty = \rho(G^\infty) \tag{42}$$

(2) For the case in which $b_{ij} = 0$ for all $(i,j) \in \Phi$, $\underline{\underline{G}}^\infty$ reaches its minimum

$$\underline{\underline{G}}^\infty_{\min} \stackrel{\text{def.}}{=} \rho(G^\infty_{\min}) \tag{43}$$

if and only if $c_o/a_o = \sqrt{\beta_{\max} \bullet \beta_{\min}}$. Equation (42) combined with equations (34) and (37) suggests that the parameter

$$\xi(G^\infty) \stackrel{\text{def.}}{=} 1 - \frac{\ln\left[2 - (G^\infty)^2\right]}{\ln\left[(G^\infty)^2\right]} \tag{44}$$

may be used to predict the numerical acceleration factor

$$\xi_r(n) \stackrel{\text{def.}}{=} \frac{[O_r(n)]_{\text{two-step procedure}}}{[O_r(2n)]_{\text{one-step procedure}}} \tag{45}$$

where $O_r(n)$ is defined in equation (I-61).

Numerical Evaluation

Initially the test problems used in the comparison of the one- and two-step methods involve the constant coefficient finite difference equations defined by equations (I-6) and (I-8). These problems were designed such that many key results of the current theoretical development could be tested numerically under the most ideal conditions. As a preliminary a line of arguments similar to that given in appendix A of reference 1 is used to obtain the following results:

(1) Let

$$h_{i,j} = h_{i+K,j} = h_{i,j+L} \qquad (i,j = 0, \pm 1, \pm 2,\ldots) \tag{46}$$

and

$$\sum_{i=0}^{(K-1)} \sum_{j=0}^{(L-1)} h_{i,j} = 0 \tag{47}$$

where $K \geq 2$ and $L \geq 2$ are two arbitrary integers. Then $u_{i,j}$'s are uniquely determined by equation (I-6) and the following auxiliary conditions:

$$u_{i,j} = u_{i+K,j} = u_{i,j+L} \qquad (i,j = 0, \pm 1, \pm 2,\ldots) \tag{48}$$

and

$$\sum_{i=0}^{(K-1)} \sum_{j=0}^{(L-1)} u_{i,j} = 0 \tag{49}$$

(2) The unique solution to equations (I-6), (48), and (49) is explicitly given by

$$u_{i,j} = \sum_{(k,\ell)\in\Psi} \frac{H^{(k,\ell)}}{\sigma_q^{(k,\ell)}} \varphi_{i,j}^{(k,\ell)} \qquad (i,j = 0, \pm 1, \pm 2,\ldots) \tag{50}$$

The only parameter in equation (50) which was not defined previously is

$$H^{(k,\ell)} \overset{\text{def.}}{=} \sum_{i=0}^{(K-1)} \sum_{j=0}^{(L-1)} h_{i,j} \overline{\varphi_{i,j}^{(k,\ell)}} \qquad (k,\ell) \in \Psi \tag{51}$$

where $\overline{\varphi_{i,j}^{(k,\ell)}}$ is the complex conjugate of $\varphi_{i,j}^{(k,\ell)}$.

For the test problems defined in table I the $h_{i,j}$'s are chosen to meet the conditions (46) and (47). They are given by either

$$h_{i,j} = \frac{\sqrt{KL}}{4}\left[\varphi_{i,j}^{(1,1)} + \varphi_{i,j}^{(K-1,1)} + \varphi_{i,j}^{(1,L-1)} + \varphi_{i,j}^{(K-1,L-1)}\right]$$

$$\equiv \cos\left(\frac{2\pi i}{K}\right)\cos\left(\frac{2\pi j}{L}\right) \tag{52}$$

or

$$h_{i,j} = \sqrt{KL} \sum_{(k,\ell)\in\Psi} \varphi_{i,j}^{(k,\ell)}$$

$$\equiv \sum_{(k,\ell)\in\Psi} \cos\left(\frac{2\pi k \cdot i}{K}\right)\cos\left(\frac{2\pi \ell \cdot j}{L}\right) \tag{53}$$

The $w_{i,j}^n$'s and $u_{i,j}^n$'s are assumed to satisfy the periodic and uniqueness conditions given in equations (48) and (49). Moreover, it is assumed that (1) $a = c = a_o = c_o = 1$, (2) $\Delta x = \Delta y = 1/K = 1/L$, and (3) the relaxation factors τ^* and $\underline{\underline{\tau}}^*$, respectively, are used in the one- and two-step procedures. Note that equations (I-38) and (I-41) coupled with assumption (1) yield

$$\tau^* = \tau^o = 1.$$

Problems 1 to 4 are studied first. Since $u_{i,j}^0 = 0$ for every i and j, equations (50) to (52) can be used to show that the only surviving $E^{0,(k,\ell)}$'s are $E^{0,(1,1)}$, $E^{0,(K-1,1)}$, $E^{0,(1,L-1)}$, and $E^{0,(K-1,L-1)}$. Moreover, since $K = L$,

$$\gamma^{(1,1)} = \gamma^{(K-1,L-1)} = \begin{Bmatrix} \gamma_{\max} & \text{if} \;\; b \geq 0 \\ \gamma_{\min} & \text{if} \;\; b \leq 0 \end{Bmatrix} \tag{54}$$

and

TABLE I.—DEFINITIONS OF PROBLEMS 1 TO 8 AND VALUES OF KEY PARAMETERS

[$a = c = a_o = c_o = 1$, $\Delta x = \Delta y = 1/K = 1/L$.]

Problem	$h_{i,j}$	b	$K=L$	$-\log_{10}(G^*)$	$-\log_{10}(G^o)$	$-\log_{10}(\underline{\underline{G}}^*)$	$-\log_{10}(1-\underline{\underline{\tau}}^*\, \underline{\underline{\gamma}}_{\min})$	$\xi(G^*)$	ξ'
1	eq. (52)	0.25	16	0.6020600	0.6189121	1.491362	1.561608	1.238549	1.261575
2	↓	.25	64	.6020600	.6031069	1.491362	1.495559	1.238549	1.239879
3		.875	16	.05799195	.07484407	.2074310	.2776769	1.788447	1.855036
4		.875	64	.05799195	.05903883	.2074310	.2116287	1.788447	1.792284
5	eq. (53)	.25	16	.6020600	.6189121	1.491362	1.561608	1.238549	1.261575
6	↓	.25	64	.6020600	.6031069	1.491362	1.495559	1.238549	1.239879
7		.875	16	.05799195	.07484407	0.2074310	0.2776769	1.788447	1.855036
8		.875	64	.05799195	.05903883	0.2074310	0.2116287	1.788447	1.792284

$$\gamma^{(K-1,1)} = \gamma^{(1,L-1)} = \begin{Bmatrix} \gamma_{\min} & \text{if} & b \geq 0 \\ \gamma_{\max} & \text{if} & b \leq 0 \end{Bmatrix} \tag{55}$$

These considerations coupled with other equations given previously lead to a simple formula for the residual norm of the one-step procedure:

$$\|r^n\| \overset{\text{def.}}{=} \left\{ \sum_{i=0}^{(K-1)} \sum_{j=0}^{(L-1)} \left[\tilde{Q}\left(e_{i,j}^{n}\right) \right]^2 \right\}^{1/2} = \frac{K}{2}(G^{\circ})^n$$

$$(K = L) \tag{56}$$

where G° is the parameter defined in equation (I-27). Thus, one concludes that in the absence of roundoff error the relation between $O_r(n)$ and n for problems 1 to 4 are represented by straight lines if the one-step method is used. The slope of each straight line is $-\log_{10}(G^{\circ})$.

Similarly by using the fact that

$$\begin{aligned} \underline{\underline{\gamma}}^{(1,1)} &= \underline{\underline{\gamma}}^{(K-1,1)} \\ &= \underline{\underline{\gamma}}^{(1,L-1)} \\ &= \underline{\underline{\gamma}}^{(K-1,L-1)} \\ &= \underline{\underline{\gamma}}_{\min} \qquad (K = L) \end{aligned} \tag{57}$$

one concludes that for the two-step procedure

$$\|r^n\| = \frac{K}{2}\left(1 - \underline{\underline{\tau}}^{*}\, \underline{\underline{\gamma}}_{\min}\right)^n \tag{58}$$

Thus, in the absence of roundoff error the relation between $O_r(n)$ and n for problems 1 to 4 are also represented by straight lines if the two-step method is used. The slope of each straight line is $-\log_{10}(1 - \underline{\underline{\tau}}^{*}\, \underline{\underline{\gamma}}_{\min})$.

The predictions given by equations (56) and (58) are confirmed by the numerical results shown in figures 2 and 3. The slopes of the upper two curves in figure 2 and all four curves in figure 3 agree with the predicted values for at least the first seven significant digits. (The accuracy of the computation is double precision on the IBM 370.) This is also true for the lower two curves in figure 2 before the roundoff error becomes dominant. Furthermore, these two curves quickly settle into horizontal lines as soon as the roundoff error becomes dominant.

These numerical results indicate that the roundoff errors never grow during the entire convergence histories of problems 1 to 4. This is also consistent with our theoretical development. Recall that a roundoff error introduced at any stage of the iterations can be considered as a linear combination of

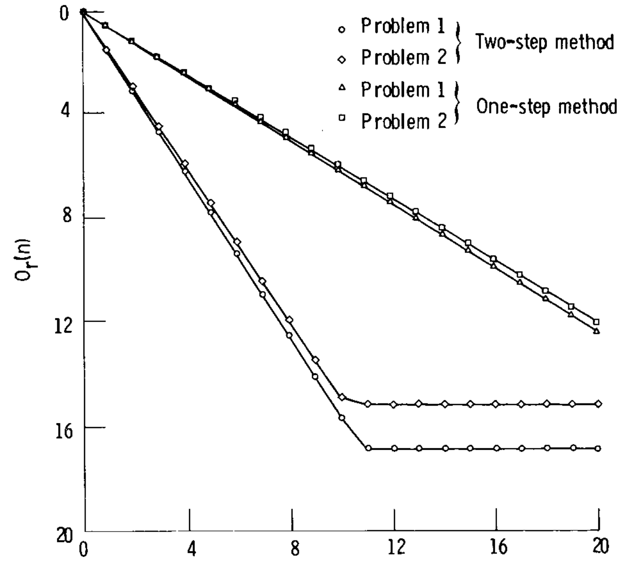

Figure 2.—Convergence histories of problems 1 and 2.

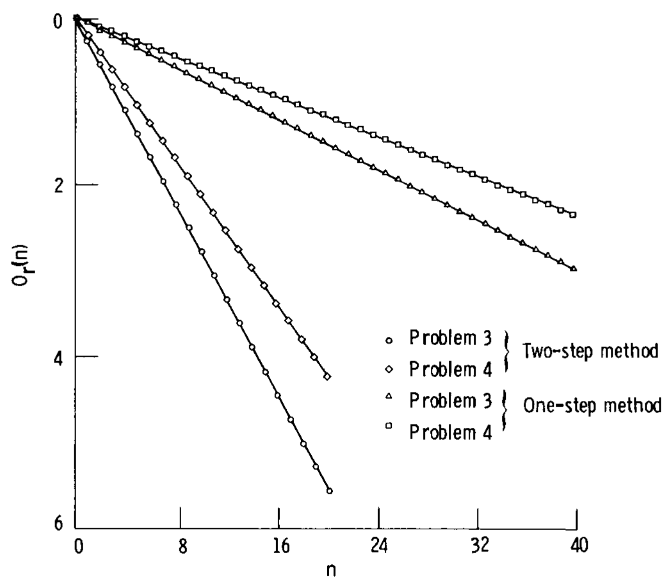

Figure 3.—Convergence histories of problems 3 and 4.

$\varphi_{i,j}^{(k,\ell)}$'s. Because of the uniqueness condition (I-A12), the $k=0$ and $\ell=0$ component of this combination is annihilated during the next iteration. On the other hand, each of the remaining components is multiplied by either $G^{(k,\ell)}(\tau^*)$ (one-step method) or $\underline{\underline{G}}^{(k,\ell)}(\underline{\underline{\tau}}^{*})$ (two-step method) as the iteration number n increases by 1. With the aid of equations (I-33), (I-35), (30), and (32), it can be shown that

$$\left|G^{(k,\ell)}(\tau^*)\right| < 1 \text{ and } \left|\underline{\underline{G}}^{(k,\ell)}(\underline{\underline{\tau}}^{*})\right| < 1 \qquad (k,\ell) \in \Psi$$

For problems 1 to 4, the acceleration factor $\xi_r(n)$ defined in equation (45) is virtually equal to

$$\xi' \overset{\text{def.}}{=} \frac{\log_{10}(1 - \underline{\underline{\tau}}^{*} \underline{\underline{\gamma}}_{\min})}{2 \log_{10}(G^{o})} \tag{59}$$

before the roundoff error becomes dominant. The value of ξ' as well as the values of five other parameters are listed in the last six columns of table I. These parameters, according to equations (I-34) and (31), are related by the following limit equations:

$$\lim_{K,L\to+\infty} \log_{10}(G^{o}) = \log_{10}(G^{*}) \tag{60}$$

$$\lim_{K,L\to+\infty} \log_{10}\left(1 - \underline{\underline{\tau}}^{*} \underline{\underline{\gamma}}_{\min}\right) = \log_{10}(\underline{\underline{G}}^{*}) \tag{61}$$

and

$$\lim_{K,L\to+\infty} \xi' = \xi(G^{*}) \tag{62}$$

Note that the parameters on the left sides of equations (60) to (62) depend on the aspect ratio $\Delta y/\Delta x$ but not on the individual values of Δx and Δy. Thus, the variation of Δx and Δy is allowable as the integers K and L approach infinity as long as the ratio $\Delta y/\Delta x$ is held constant. Since $\Delta y/\Delta x = 1$ for problems 1 to 8, one may expect that the values of the parameters on the left sides of equations (60) to (62) approach more closely to the values of the corresponding grid-independent parameters on the right sides as the values of K and L increase from $K = L = 16$ to $K = L = 64$. The values shown in table I confirm this expectation.

As also shown in table I, the values of $-\log_{10}(G^{o})$ and $-\log_{10}(1 - \underline{\underline{\tau}}^{*} \underline{\underline{\gamma}}_{\min})$, and thus the actual convergence rates of the one- and two-step procedures, may be substantially underestimated by the values of $-\log_{10}(G^{*})$ and $-\log_{10}(\underline{\underline{G}}^{*})$, respectively, if b is relatively large, and K and L are relatively small. As a result the convergence rates tend to be more sensitive to the change of the integers K and L if the value of $b/\sqrt{ac}$ is closer to 1. (See fig. 3.)

For problems 5 to 8 the $h_{i,j}$'s are specified according to equation (53). With this choice of the source term all $E^{0,(k,\ell)}$'s survive. As a result the relation between $O_r(n)$ and n for problems 5 to 8 are no longer represented by straight lines. However, as expected from theoretical considerations, the slope of any curve shown in figures 4 and 5 approaches either $-\log_{10}(G^{o})$ (one-step procedure) or $-\log_{10}[\underline{\underline{G}}(\underline{\underline{\tau}}^{*})]$ (two-step procedure) before the roundoff error becomes dominant. Note that $\underline{\underline{G}}(\underline{\underline{\tau}}^{*}) = \underline{\underline{G}}^{*}$ if $\hat{a}' = \hat{c}'$.

The initial comparisons of the one- and two-step methods in regard to their ability to solve PDE's with variable coefficients involve problems 1 to 17 of reference 1. The relative efficiencies of these two methods, measured in terms

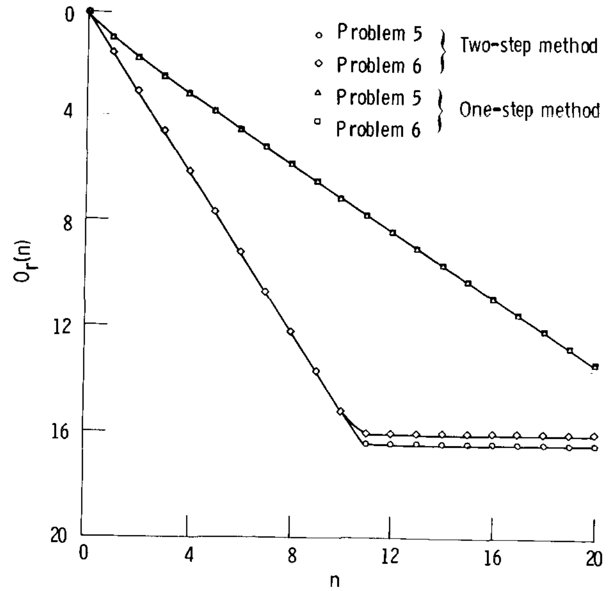

Figure 4.—Convergence histories of problems 5 and 6.

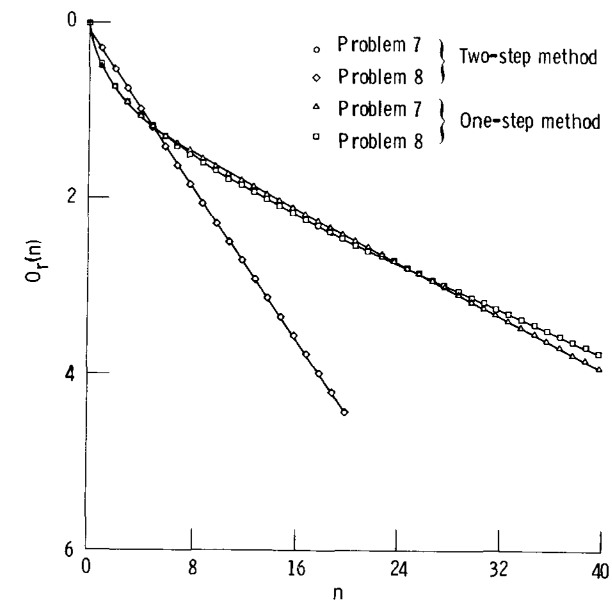

Figure 5.—Convergence histories of problems 7 and 8.

of the parameter $\xi_r(n)$ (eq. (45)), are given in table II. It is seen that (1) the convergence is accelerated, that is, $\xi_r(n) > 1$, by the two-step procedure in only six test cases, and (2) without any exception, $\xi_r(n)$ is smaller than the corresponding theoretical parameter $\xi(G^{\infty})$, and the discrepancy is rather large for the test problems with rapidly varying coefficients, that is, problems 13 to 15 of reference 1. These disappointing results, however, are not surprising because of the following considerations: (1) the technique of local relaxation, obviously, is less viable in the case of the

TABLE II.—VALUES OF $\xi(G^{\infty})$ AND $\xi_r(n)$ FOR PROBLEMS 1 TO 17 OF REFERENCE 1

[For problems 1 to 5, $n = 10$; for problems 6 to 15, $n = 16$; and for problems 16 and 17, $n = 5$.]

	Problem								
	1	2	3	4	5	6	7	8	9
$\xi(G^{\infty})$	1.234	1.237	1.228	1.234	1.236	1.402	1.403	1.394	1.403
$\xi_r(n)$	1.077	1.133	1.144	0.904	1.024	0.962	1.068	0.730	0.977
	Problem								
	10	11	12	13	14	15	16	17	
$\xi(G^{\infty})$	1.403	1.402	1.289	1.289	1.289	1.289	1.336	1.367	
$\xi_r(n)$	0.897	0.804	0.809	0.521	0.347	0.169	0.793	1.216	

two-step procedure, and (2) the one-step method convergence rates associated with these test problems are all relatively high, and thus the advantage of using the two-step procedure is greatly reduced.

To demonstrate that the two-step method could be substantially faster than the one-step method for the test problems with low one-step method convergence rate, problems 9 and 10 are introduced, which are modified versions of problems 16 and 17 of reference 1. The modification involves only the enlargement of the domain of equation (I-69) from $1 \geq x \geq 0$ and $1 \geq y \geq 0$ to $1.5 \geq x \geq 0$ and $1.5 \geq y \geq 0$. A comparison between table II of reference 1 and table III of this report reveals that this simple modification results in a large reduction in the values of $O_t(10)$ and thus the one-step method convergence rates. Furthermore, it can be seen that the two-step method, as indicated by the values of $\xi_r(5)$ and $\xi_r(10)$, is indeed substantially faster than the one-step method for problems 9 and 10.

Problems 18 and 19 defined in reference 1 are associated with a self-adjoint PDE (I-70) in which the coefficients p and q are identical. As noted in the section Local Relaxation, for these test problems the two-step method is inferior to the one-step method.

The next test problems to be discussed are those defined in table III of reference 1. If the values of c_o/a_o used in the iterations are chosen according to equation (I-54), the computational efficiencies of the one-step and two-step methods are about equal, as shown in table IV. It is also shown that for the test problem associated with equation (I-74) the convergence rates are sharply reduced if $c_o/a_o = 1$ is assumed in the iterations. In this case the computational efficiency of the two-step method is about twice that of the one-step method.

Finally, the one- and two-step methods are compared by using the three-dimensional test problem defined in the section Application to a 3-D Flow Problem of reference 1. As in

TABLE III.—VALUES OF KEY PARAMETERS FOR PROBLEMS 9 AND 10

Problem	c_o/a_o	$O_t(10)$	$\xi(G^{\infty})$	$\xi_r(5)$	$\xi_r(10)$
9	[a]0.1239	1.083	1.654	2.009	1.840
10	[a]0.1065	.928	1.698	1.741	1.745

[a]Evaluated from eq. (I-54).

TABLE IV.—VALUES OF KEY PARAMETERS FOR TEST PROBLEMS DEFINED IN TABLE III OF REFERENCE 1

Equation	Solution method	c_o/a_o	T_t, sec
(I-73)	One-step	[a]0.8839	1.871
(I-73)	Two-step	[a].8839	1.531
(I-74)	One-step	[a]9.989	.888
	Two-step	[a]9.989	1.050
	One-step	1.0	14.04
	Two-step	1.0	7.61

[a]Evaluated from eq. (I-54).

reference 1 it is assumed that $p_1 = p_2 = 1$ and $p_3 = 0.4135$. The values of $\xi_r(4)$ obtained during the 25 passes through the inner loop range from 1.140 to 1.308, with the average being 1.256.

Concluding Remarks

A two-step semidirect procedure was developed to accelerate the one-step procedure described in reference 1. The acceleration may be substantial for elliptic problems which have low convergence rates with the one-step procedure.

A key element in the development of the two-step procedure is to choose the coefficients a', b', and c' such that the convergence rate (in a sense defined in the section Analysis) can be maximized. This optimization problem is solved by equation (29). With the coefficients a', b', and c' so chosen a simple monotonic relation exists between the asymptotic error multiplication factors for the one- and two-step procedures. This relation not only enables us to establish the superiority of the two-step procedure compared with the one-step procedure, but also contributes greatly to the simplicity of the two-step procedure.

Finally, it should be emphasized that the development of the current one- and two-step procedures involves many bold assumptions. In future development it is hoped that the validity of these assumptions may be evaluated by using a rigorous matrix formulation. It is also hoped that the limitations imposed by these assumptions can be at least partially removed.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, February 6, 1986

Appendix—Mathematical Foundation for the section Analysis

The existence of the supremum $\underline{\underline{\Sigma}}^{\infty}$ defined in equation (25) is shown here. With the aid of equations (I-B18) and (18), equations (15), (21), and (24) imply that

$$\frac{\lambda_{max} \bullet \lambda'_{max}}{\lambda_{min} \bullet \lambda'_{min}} \geq \underline{\underline{\Sigma}} \tag{A1}$$

Since the upper bound of $\underline{\underline{\Sigma}}$ given in equation (A1) is independent of the integers K and L, the existence of $\underline{\underline{\Sigma}}^{\infty}$ is established.

To prove that (1) $\underline{\underline{\Sigma}}^{\infty} \geq \underline{\underline{\Sigma}}^{*}$ and (2) $\underline{\underline{\Sigma}}^{\infty} = \underline{\underline{\Sigma}}^{*}$ if and only if eq. (27) is satisfied, the following Lemmas are established:

Lemma 1

Let

$$H(v_1,v_2) \overset{\text{def.}}{=} [\hat{a}(v_1)^2 + \hat{c}(v_2)^2 + 2\hat{b}v_1v_2] \; [\hat{a}'(v_1)^2 + \hat{c}'(v_2)^2 + 2\hat{b}'v_1v_2] \tag{A2}$$

where v_1 and v_2 are real variables satisfying

$$(v_1)^2 + (v_2)^2 = 1 \tag{A3}$$

Then the supremum H_{max} and the infimum H_{min} of the function H over its domain exist. Furthermore, $H_{max} \geq H_{min} > 0$, and there exist real members v_1^+, v_2^+, v_1^-, and v_2^-, such that

$$(v_1^+)^2 + (v_2^+)^2 = (v_1^-)^2 + (v_2^-)^2 = 1 \tag{A4}$$

$$H(v_1^+,v_2^+) = H_{max} > 0 \tag{A5}$$

and

$$H(v_1^-,v_2^-) = H_{min} > 0 \tag{A6}$$

Proof

Since H is continuous over a compact domain, H_{max}, H_{min}, v_1^+, v_2^+, v_1^-, and v_2^- must exist. It follows from equations (I-4) and (16) that $H_{max} \geq H_{min} > 0$.

Lemma 2

$$\underline{\underline{\Sigma}}^{\infty} \geq \frac{H_{max}}{H_{min}} \tag{A7}$$

Proof

Let

$$\underline{\underline{F}}(s_1,s_2,t_1,t_2) \overset{\text{def.}}{=} [\hat{a}(s_1)^2 + \hat{c}(s_2)^2 + 2\hat{b}s_1s_2t_1t_2] \; [\hat{a}'(s_1)^2 + \hat{c}'(s_2)^2 + 2\hat{b}'s_1s_2t_1t_2] \tag{A8}$$

where s_1, s_2, t_1, and t_2 are real variables satisfying equations (I-B5) and (I-B7). Using equations (11), (12), (15), and (I-B13) to (I-B17), one concludes that

$$\underline{\underline{\gamma}}^{(k,\ell)} = \underline{\underline{F}}(s_x,s_y,t_x,t_y) \qquad (k,\ell) \in \Psi \tag{A9}$$

Furthermore, a comparison between equations (A2) and (A8) reveals that

$$H(v_1,v_2) = \underline{\underline{F}}\left(|v_1|, |v_2|, \frac{v_1}{|v_1|}, \frac{v_2}{|v_2|}\right) \quad \text{if } v_1 \neq 0 \text{ and } v_2 \neq 0 \tag{A10}$$

Let v_1 and v_2 be two given real numbers satisfying (1) $(v_1)^2 + (v_2)^2 = 1$, and (2) $v_1 \neq 0$ and $v_2 \neq 0$. Following a line of arguments (eqs. (I-B21) to (I-B31)), which was used in reference 1 to establish the existence of the integers K_o and L_o, one can show that for any $\delta_x > 0$, $\delta_y > 0$, $\epsilon_x > 0$, and $\epsilon_y > 0$ there exists a pair of integers K_o and L_o such that for any $K \geq K_o$ and $L \geq L_o$ two integers k and ℓ can be found to satisfy the requirements

$$\delta_x > \big| s_x - |v_1| \big|$$

$$\delta_y > \big| s_y - |v_2| \big|$$

$$\epsilon_x > \left| t_x - \frac{v_1}{|v_1|} \right|$$

$$\epsilon_y > \left| t_y - \frac{v_2}{|v_2|} \right|$$

Thus, in the case having $v_1^+ \neq 0$, $v_2^+ \neq 0$, $v_1^- \neq 0$, and $v_2^- \neq 0$ equations (A9) and (A10) along with the continuity of the function $\underline{\underline{F}}$ can be used to show that for any $\xi > 0$ there exists a pair of integers K and L large enough that $(k,\ell) \in \Psi$ and $(k',\ell') \in \Psi$ can be found to satisfy the requirement

$$\xi > \left| \frac{\underline{\underline{\gamma}}^{(k,\ell)}}{\underline{\underline{\gamma}}^{(k',\ell')}} - \frac{H(\nu_1^+,\nu_2^+)}{H(\nu_1^-,\nu_2^-)} \right|$$

With the aid of equations (24) and (25), one concludes that inequality (A7) is true if $\nu_1^+ \neq 0$, $\nu_2^+ \neq 0$, $\nu_1^- \neq 0$, and $\nu_2^- \neq 0$. Since $H(0, \pm 1) = \hat{c}\hat{c}' = \underline{\underline{\gamma}}^{(0,\ell)}$, and $H(\pm 1, 0) = \hat{a}\hat{a}' = \underline{\underline{\gamma}}^{(k,0)}$, inequality (A7) is valid for all ν_1^+, ν_2^+, ν_1^-, and ν_2^- which satisfy equations (A4) to (A6). QED.

Lemma 3

Let

$$f(\theta) \overset{\text{def.}}{=} [\lambda_1\theta + \lambda_2(1-\theta)][\lambda_1'\theta + \lambda_2'(1-\theta)] > 0 \qquad 1 \geq \theta \geq 0 \tag{A11}$$

where λ_1, λ_2, λ_1', and λ_2' are given positive numbers. Then

(1) The supremum f_{max} and the infimum f_{min} of the function f over its domain exist, and $f_{max} \geq f_{min} > 0$.

(2) $\dfrac{f_{max}}{f_{min}} \geq \dfrac{f(1/2)}{\text{Min}\ \{f(0), f(1)\}} \geq \dfrac{(\lambda_1 + \lambda_2)^2}{4\lambda_1\lambda_2}$

(3) $\dfrac{f_{max}}{f_{min}} = \dfrac{(\lambda_1 + \lambda_2)^2}{4\lambda_1\lambda_2}$ if and only if $\lambda_1\lambda_1' = \lambda_2\lambda_2'$

Proof

Part (1) is obvious. To facilitate the proof of (2) and (3), three exclusive cases are studied separately.

Case 1. $\lambda_1\lambda_1' = \lambda_2\lambda_2'$.—For this case

$$f(\theta) = \lambda_2\lambda_2'[\lambda_1\theta + \lambda_2(1-\theta)]\left[\frac{\theta}{\lambda_1} + \frac{1-\theta}{\lambda_2}\right]$$

and thus

$$f(1/2) = \frac{\lambda_2\lambda_2'(\lambda_1 + \lambda_2)^2}{4\lambda_1\lambda_2} \geq f(\theta) \geq f(0)$$

$$= f(1) = \lambda_2\lambda_2' \qquad 1 \geq \theta \geq 0$$

As a result

$$\frac{f_{max}}{f_{min}} = \frac{f(1/2)}{f(0)}$$

$$= \frac{f(1/2)}{f(1)}$$

$$= \frac{(\lambda_1 + \lambda_2)^2}{4\lambda_1\lambda_2}$$

Case 2. $\lambda_1\lambda_1' > \lambda_2\lambda_2'$.—For this case Min $\{f(0), f(1)\} = f(0)$, and

$$\frac{f(1/2)}{f(0)} - \frac{(\lambda_1 + \lambda_2)^2}{4\lambda_1\lambda_2} = \frac{(\lambda_1 + \lambda_2)(\lambda_1\lambda_1' - \lambda_2\lambda_2')}{4\lambda_1\lambda_2\lambda_2'} > 0$$

Case 3. $\lambda_2\lambda_2' > \lambda_1\lambda_1'$.—For this case Min $\{f(0), f(1)\} = f(1)$, and

$$\frac{f(1/2)}{f(1)} - \frac{(\lambda_1 + \lambda_2)^2}{4\lambda_1\lambda_2} = \frac{(\lambda_1 + \lambda_2)(\lambda_2\lambda_2' - \lambda_1\lambda_1')}{4\lambda_1\lambda_2\lambda_1'} > 0$$

QED

Lemma 4

$$\frac{H_{max}}{H_{min}} \geq \underline{\underline{\Sigma}}^*$$

with the understanding that the equality sign is valid if and only if equation (27) is satisfied.

Proof

To proceed, the first quadratic form on the right side of equation (A2) is diagonalized (ref. 3) by using an orthogonal transformation

$$(\nu_1, \nu_2) \rightarrow (\underset{\sim}{\nu_1}, \underset{\sim}{\nu_2}).$$

Thus,

$$(\underset{\sim}{\nu_1})^2 + (\underset{\sim}{\nu_2})^2 = (\nu_1)^2 + (\nu_1)^2 = 1 \tag{A12}$$

and

$$H(\nu_1,\nu_2) = \underset{\sim}{H}(\underset{\sim}{\nu_1}, \underset{\sim}{\nu_2}) \overset{\text{def.}}{=} \left[\lambda_{max}(\underset{\sim}{\nu_1})^2 + \lambda_{min}(\underset{\sim}{\nu_2})^2\right] \times \left[\underset{\sim}{\hat{a}}'(\underset{\sim}{\nu_1})^2 + \underset{\sim}{\hat{c}}'(\underset{\sim}{\nu_2})^2 + 2\underset{\sim}{\hat{b}}'\,\underset{\sim}{\nu_1}\,\underset{\sim}{\nu_2}\right] \tag{A13}$$

where λ_{max} and λ_{min} are defined in equations (I-30) and (I-31). Let

$$\underset{\sim}{\hat{D}} \overset{\text{def.}}{=} \begin{pmatrix} \lambda_{max} & 0 \\ 0 & \lambda_{min} \end{pmatrix} \text{ and } \underset{\sim}{\hat{D}}' \overset{\text{def.}}{=} \begin{pmatrix} \underset{\sim}{\hat{a}}' & \underset{\sim}{\hat{b}}' \\ \underset{\sim}{\hat{b}}' & \underset{\sim}{\hat{c}}' \end{pmatrix} \tag{A14}$$

There exists an orthogonal matrix U such that

$$\underset{\sim}{\hat{D}} = U\hat{D}U^{-1} \text{ and } \underset{\sim}{\hat{D}}' = U\hat{D}'U^{-1} \tag{A15}$$

where $\hat{D}$ and $\hat{D}'$ are the matrices defined in equation (28). As a result the matrices $\underset{\sim}{\hat{D}}'$, like $\hat{D}'$, is positive definite; that is,

$$\left.\begin{array}{l} \underset{\sim}{\hat{a}}' > 0 \\ \\ \underset{\sim}{\hat{c}}' > 0 \\ \\ \underset{\sim}{\hat{a}}'\underset{\sim}{\hat{c}}' - (\underset{\sim}{\hat{b}}')^2 > 0 \end{array}\right\} \tag{A16}$$

Let

$$\underset{\sim}{f}(\theta) \overset{\text{def.}}{=} [\lambda_{\max}\theta + \lambda_{\min}(1-\theta)][\underset{\sim}{\hat{a}}'\theta + \underset{\sim}{\hat{c}}'(1-\theta)]$$

$$1 \geq \theta \geq 0 \tag{A17}$$

Then equations (A12) and (A13) imply that

$$\underset{\sim}{H}(\underset{\sim}{v}_1, \underset{\sim}{v}_2) = \underset{\sim}{f}((\underset{\sim}{v}_1)^2) + 2\underset{\sim}{\hat{b}}'\,\underset{\sim}{v}_1\underset{\sim}{v}_2$$

$$\times [\lambda_{\max}(\underset{\sim}{v}_1)^2 + \lambda_{\min}(\underset{\sim}{v}_2)^2] \tag{A18}$$

To proceed further, two exclusive cases, (1) $\underset{\sim}{\hat{b}}' = 0$ and (2) $\underset{\sim}{\hat{b}}' \neq 0$, are studied separately.

Case 1. $\underset{\sim}{\hat{b}}' = 0$.—For this case $\underset{\sim}{H}(\underset{\sim}{v}_1, \underset{\sim}{v}_2) = \underset{\sim}{f}((\underset{\sim}{v}_1)^2)$. With the aid of equations (A5), (A6), (A12) to (A16), (26), and (I-33) Lemma 3 implies that

$$\frac{H_{\max}}{H_{\min}} \geq \underset{=}{\Sigma}^*$$

with the understanding that the equality sign is valid if and only if equation (27) is satisfied.

Case 2. $\underset{\sim}{\hat{b}}' \neq 0$.—For this case, equation (27) is violated since $\underset{\sim}{\hat{D}}\underset{\sim}{\hat{D}}'$, and thus $\hat{D}\hat{D}'$, can not be a scalar matrix. Furthermore,

$$\underset{\sim}{H}\left(\frac{1}{\sqrt{2}}\frac{\underset{\sim}{\hat{b}}'}{|\underset{\sim}{\hat{b}}'|}, \frac{1}{\sqrt{2}}\right) = \underset{\sim}{f}\left(\frac{1}{2}\right) + \frac{|\underset{\sim}{\hat{b}}'|}{2}(\lambda_{\max} + \lambda_{\min})$$

$$> \underset{\sim}{f}\left(\frac{1}{2}\right)$$

and

$$\underset{\sim}{H}(0,1) = \underset{\sim}{f}(0)$$

$$\underset{\sim}{H}(1,0) = \underset{\sim}{f}(1)$$

Thus, with the aid of Lemma 3 one concludes that

$$\frac{H_{\max}}{H_{\min}} > \frac{\underset{\sim}{f}(1/2)}{\text{Min}\,\{\underset{\sim}{f}(0), \underset{\sim}{f}(1)\}} \geq \underset{=}{\Sigma}^* \qquad \text{QED}$$

Lemma 5

Let s_1, s_2, t_1, and t_2 be real variables satisfying equations (I-B5) and (I-B7). Then

$$\Lambda\underset{=}{\Sigma}^* \geq \underset{=}{F}(s_1,s_2,t_1,t_2) \geq \Lambda$$

if the matrices $\hat{D}$ and $\hat{D}'$ are related by equation (27). Lemma 5 is a special case of theorem 2 in reference 4.

Lemmas 2 and 4 imply that (1) $\underset{=}{\Sigma}^\infty \geq \underset{=}{\Sigma}^*$ and (2) $\underset{=}{\Sigma}^\infty > \underset{=}{\Sigma}^*$ if the condition (27) is violated. On the other hand, if condition (27) is satisfied, Lemma 5 combined with equations (A9), (24), and (25) implies that $\underset{=}{\Sigma}^* \geq \underset{=}{\Sigma}^\infty$. Thus, one concludes that $\underset{=}{\Sigma}^* = \underset{=}{\Sigma}^\infty$ if and only if condition (27) is satisfied.

Finally, expressions (30) and (31) are shown as follows: If the matrices $\hat{D}$ and $\hat{D}'$ are related by equation (27) with $\Lambda = 1$, Lemmas 4 and 5 coupled with equations (A9) and (A10) imply that

$$\underset{=}{\Sigma}^* = H_{\max} \geq \underset{=}{\gamma}^{(k,\ell)} \geq H_{\min} = 1 \qquad (k,\ell) \in \Psi \tag{A19}$$

(Eq. (A10) may be replaced by $H(v_1,v_2) = \underset{=}{F}(v_1,v_2,0,0)$ if either $v_1 = 0$ or $v_2 = 0$.) Expression (30) follows directly from equation (A19). Furthermore, with the aid of expression (A19), equation (31) can be shown by using a line of arguments similar to that presented in the proof of Lemma 2.

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16. Abstract

A two-step semidirect procedure is developed to accelerate the one-step procedure described in NASA TP-2529. For a set of constant coefficient model problems, the acceleration factor increases from 1 to 2 as the one-step procedure convergence rate decreases form $+\infty$ to 0. It is also shown numerically that the two-step procedure can substantially accelerate the convergence of the numerical solution of many partial differential equations (PDE's) with variable coefficients.

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